

Quininic acid
86-68-0 | DTXSID70323339

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 323 °C

Global applicability domain: Inside

Local applicability domain index: 2.82e-01

Confidence level: 6.34e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Chloramben</div> <div>Measured: 312</div> <div>Predicted: 301</div>	<div>Image not found</div> <div>Benzoic acid, 2-phenoxy-</div> <div>Measured: 355</div> <div>Predicted: 325</div>	<div>Image not found</div> <div>2,4-DB</div> <div>Measured: 324</div> <div>Predicted: 306</div>
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